Erratum: Covalent Bonding of CN to the Pt(111) Surface [Phys. Rev. Lett. 80, 766 (1998)]

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The CN/Pt(111) vibrational spectrum presented in Fig. 1 of our Letter is incorrect. We used a new procedure for CN adsorption which, as we learned later on, seemed to allow for a large CO contamination of the surface [1]. Here we present a corrected Fig. 1, containing a spectrum of CN on Pt(111) which was obtained after adsorption from a solution of tetrabutylammonium cyanide in acetonitrile.

The change in the form of the spectrum does not alter the physical conclusions of the Letter, for the corrected spectrum agrees better with the theory than the incorrect one. The differences are (1) in the corrected spectrum there is no peak due to adsorption on hollow (or bridge) sites observable, which actually should have been expected because of the much smaller dynamic dipole moments for CN on these sites ($0.05e$). Only on-top adsorption of CN with a stretching frequency of 2108 cm^{-1} is observed. (2) The intensity of the CN band in the corrected spectrum is 1 order of magnitude smaller than that of CO adsorbed at on-top sites (note the different scales for CN and CO), which is consistent with the smaller dynamic dipole moment of on-top CN ($0.35e$) in comparison with CO ($1.2e$).

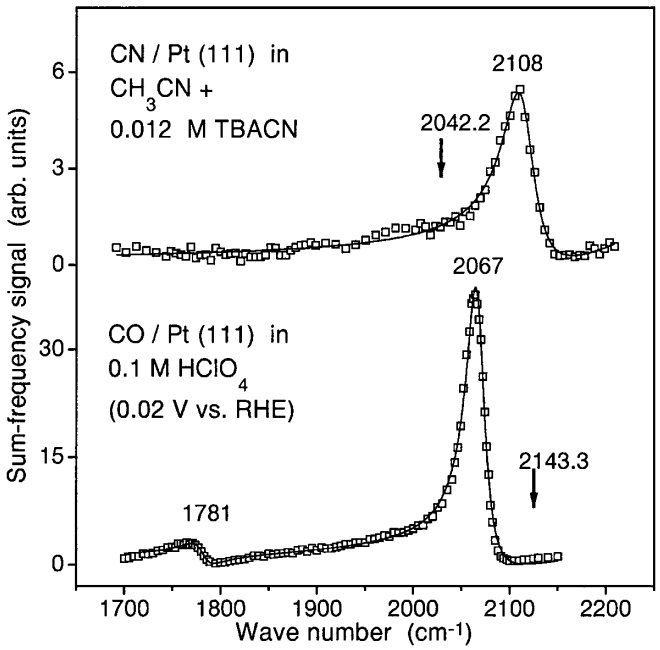

FIG. 1. Sum-frequency spectra of CN adsorbed on Pt(111) from a solution of 0.012 M tetrabutylammonium cyanide (TBACN) in acetonitrile (CH_3CN) and of CO adsorbed in an aqueous perchloric acid electrolyte. CN was adsorbed on an uncharged surface without applied potential. The arrows indicate the frequencies of the isolated molecules. The solid lines are fits to the data.

[1] F. Dederichs, A. Petukhova, and W. Daum (to be published).

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